Sustainable Transportation Program
Update

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

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# Accelerating the automotive engine through high performance computing

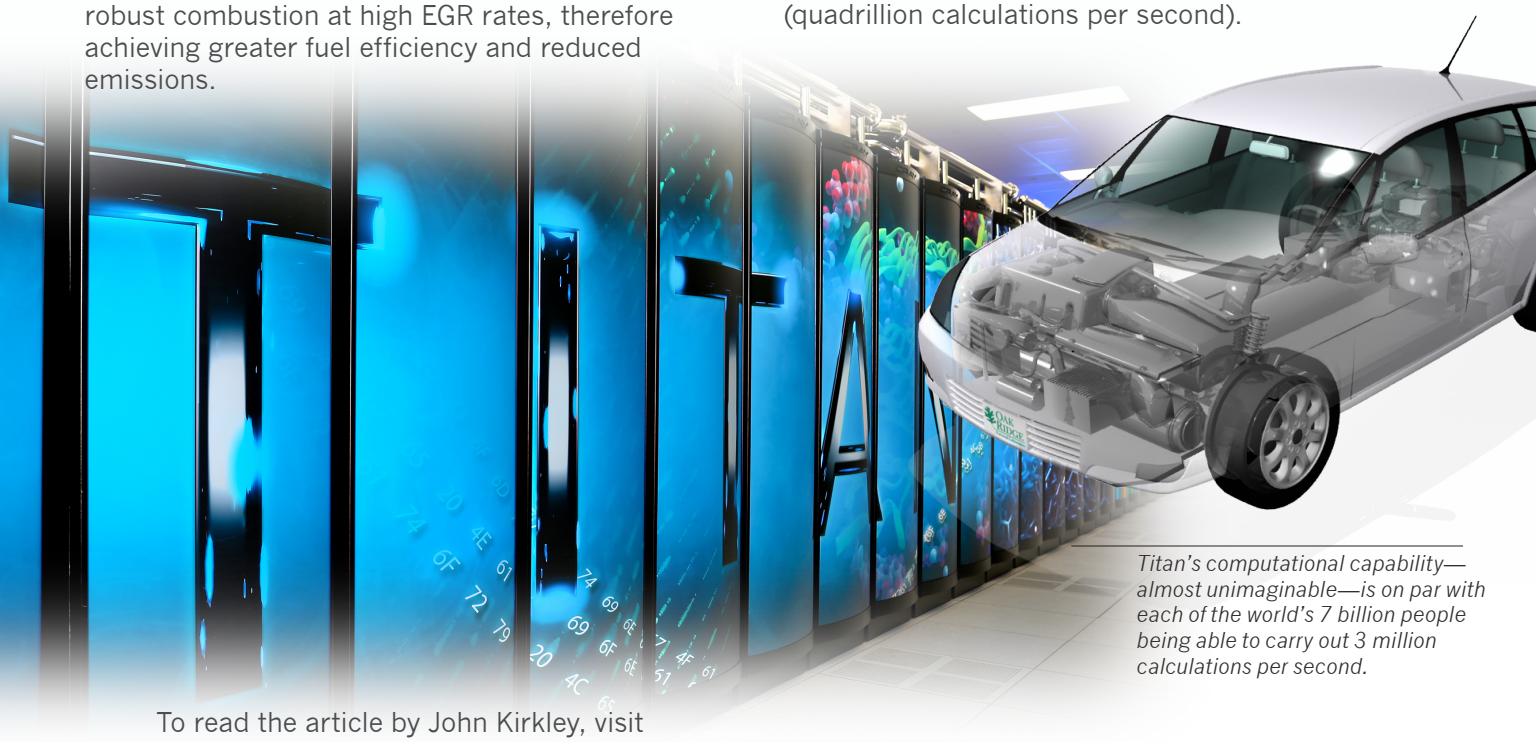
Today's automotive manufacturers are in pursuit of a more perfect internal combustion engine, one designed to meet both consumer and regulatory demands for clean and efficient operation. In a recent online article, *Digital Manufacturing Report* journalist John Kirkley sheds light on two ORNL-industry collaborations that are leveraging the lab's scientific and high performance computing (HPC) capabilities to advance engine design. Both projects are funded through the DOE Vehicle Technologies Program Advanced Combustion Engine subprogram.

The first uses high-resolution computational fluid dynamics modeling based on Large Eddy Simulation (LES) to examine stochastic and deterministic processes that drive cycle-to-cycle instabilities to improve understanding of the effects of higher exhaust gas recirculation (EGR) rates on the combustion process. The modeling facilitates enhanced engine system designs that enable robust combustion at high EGR rates, therefore achieving greater fuel efficiency and reduced emissions.

The second project's objective is to improve the understanding and design optimization of gasoline fuel injector hole patterns for improved engine efficiency and reduced emissions. Understanding spray formation and the complex fuel-air mixing within the combustion chamber is critical in obtaining higher efficiency engines. HPC offers a pathway to accurate and accelerated future design modifications.

According to FEERC's Robert Wagner, who contributed to the article, ORNL high performance computing capabilities are "absolutely essential to making the breakthroughs necessary for accelerating advanced engine design and the ability of the automotive manufacturers to meet and surpass tomorrow's stringent emission regulations."

Well positioned to address industry needs, ORNL enhanced its capabilities exponentially just days after the article posted with the launch of Titan, the world's most powerful supercomputer for open science with a theoretical peak performance exceeding 20 petaflops (quadrillion calculations per second).



*Titan's computational capability—almost unimaginable—is on par with each of the world's 7 billion people being able to carry out 3 million calculations per second.*

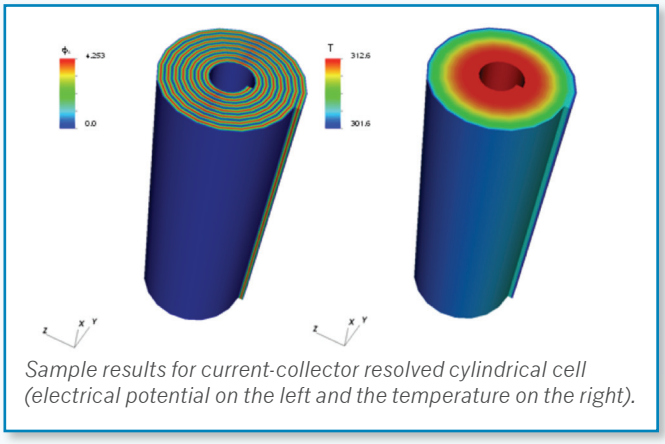
To read the article by John Kirkley, visit
http://www.digitalmanufacturingreport.com/dmr/2012-10-25/a_new_era_in_automotive_engine_development_driven_by_hpc.html?featured=top.

## Battery simulation tool released

Given the complex requirements for developing electrical energy storage devices for future transportation needs, a predictive simulation capability is needed that can guide rapid battery design by considering performance and safety implications of different chemistry and materials choices. With such models not currently in existence, the goal of the Vehicle Technology Program's Computer Aided Engineering for Batteries (CAEBAT) program is to do just that – create simulation tools for designing batteries. The program is led by the National Renewable Energy Laboratory with ORNL and several industrial partners.

Through its role with the CAEBAT project, ORNL is developing a flexible, robust, and computationally scalable open-architecture framework that enables seamless multi-scale and multi-physics simulations of battery performance and safety. The project has four main components: a) open architecture software (OAS), the base computational infrastructure; b) virtual integrated battery environment (VIBE), the OAS framework along with physics and support components and the adapters; c) BatteryML, the standard for specifying input; and d) battery state, the state file(s) to transfer information between the components.

In late October, the ORNL team released a Beta version of the CAEBAT OAS framework to industry partners. This version has all the capabilities to do electrochemical-electrical-thermal simulations of a pouch or a cylindrical cell. Watch for progress updates as the team works closely with partners in the days ahead.

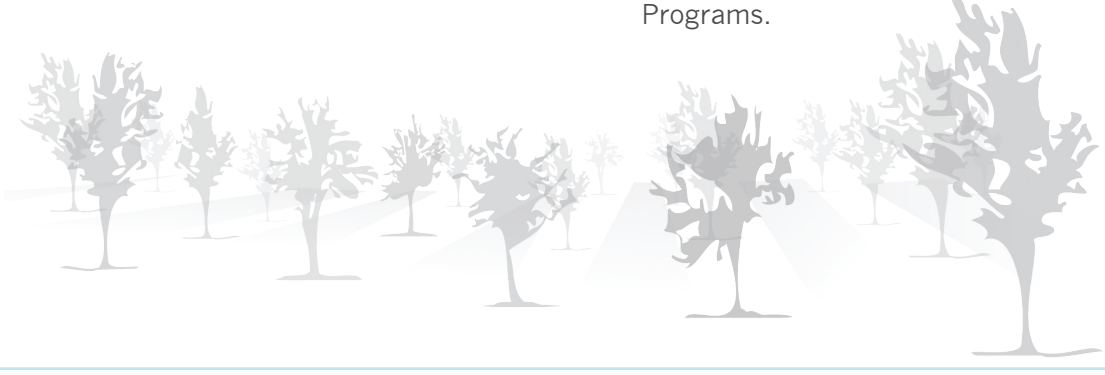



*Sample results for current-collector resolved cylindrical cell (electrical potential on the left and the temperature on the right).*

## Billion-Ton API released during Energy Datapalooza

To allow better access to Billion-Ton Update data, a team lead by ORNL researchers has developed an application programming interface (API). The API was released on October 1 at the White House's Energy Datapalooza, where more than 150 of America's entrepreneurs, software developers, energy experts, and policy makers gathered to celebrate new products, services, and apps that are advancing a secure, clean energy future—all built with freely available data from the government and other sources.

The Billion-Ton API allows developers and researchers to more easily integrate the Billion-Ton data into their models and applications without the need to host the information on their own systems. ORNL team members include Computational Sciences and Engineering Division's Aaron Myers, Sunil Movva, Budhendra Bhaduri, Rajasekar Karthik, and Phil Nugent; and Environmental Sciences Division's Laurence Eaton. The team's efforts support the Bioenergy Knowledge Discovery Framework project funded by the Office of Biomass Programs.



## Vehicle charging goes unplugged; project receives $8 million from DOE

ORNL researchers are dropping the cord in battery charging for electric vehicles and plug-in hybrid models in favor of wireless power transfer (WPT) technology that has proven to be safer, more convenient, and more efficient.

Using a proprietary design created at ORNL's National Transportation Research Center, John M. Miller, principal investigator with the lab's Power Electronics Group, and his team have developed a hands-free, magnetized coil system that wirelessly transfers electricity to a vehicle with an onboard battery pack while it's parked over a floor-embedded charging sensor.

The project's multi-phase approach includes testing stationary charging of multiple vehicles in real-world situations, such as cars and buses in parking lots and garages, and a longer-term objective of further developing dynamic in-motion charging in which the vehicle's battery pack is replenished as it is driven over sensors installed along roadways.

"This is the ultimate in convenience. Without having to use a cord to plug in the charger to the vehicle, wireless technology takes the charging burden completely off the driver, making it autonomous and safer for people to use," John said.

Test results from the lab show that using ORNL's wireless coils as a charging source can bring an EV's battery pack to fully charged with 90% efficiency, which is comparable to the current plug-in method and is the highest charge rate among competing wireless power transfer technologies for EVs.

The ORNL project team's impressive gains in wireless charging research, coupled with a strong focus on user safety, led to an $8 million award from the US Department of Energy to fund further development and demonstration of the grid-connected, ground-based coil units. With DOE's support, ORNL plans to install its latest wireless charging coil design at an existing EV charging station as part of the lab's Sustainable Campus Initiative. It will be tested with a Toyota Prius parked over an 18- to 20-inch square of charging coils that emits between 7 and 10 kilowatts of electrical charge.

John explained that during the next 3 years, his team will continue development of the static charging functionality of the wireless charging system; take the technology into the production intent phase as it moves toward commercialization; and present the wireless charging system to DOE for further testing, data collection, and validation.

ORNL has focused on WPT for onboard vehicle battery charging since 2008. During the last year, the lab has made significant strides in modified coil technology to effectively and efficiently handle in-motion charging. In the future, said John, moving from stationary to in-motion wireless charging of onboard vehicle batteries may require installation of in-ground direct current cabling along American highways. Setting up EV charging stations, which could resemble and function like toll roads, could be done in tandem with scheduled road construction and repair. EV owners could use the equivalent of an electronic "fast pass" system to pay for wireless charging as they drive over embedded sensors.

The ORNL-led team includes Evatran, General Motors, Toyota, and Clemson University.


*Researcher Steven Campbell demonstrates an electric vehicle being wirelessly charged using ORNL technology.*

## Employee Excellence

### SAE Fellow status awarded to Wagner, West

FEERC's Robert Wagner and Brian West have been elevated to Fellow status within the Society of Automotive Engineers. Letters received from the SAE Fellows Committee note that Robert's selection is based on his distinctive contributions in combustion stability fundamentals and the scaling and harmonization of low temperature combustion processes to multi-cylinder engines, while Brian's selection is attributed to outstanding research accomplishments that have impacted multiple national fuel policies and sustained, unique contributions to technology and data supporting improved vehicle fuel economy. The two will be honored during the SAE World Congress and Exhibition in Detroit in April.

*Brian West*

*Robert Wagner*

- CTA's David Greene has been selected as the 2012 recipient of Transportation Research Board's (TRB) Roy W. Crum Distinguished Service Award. An ORNL Corporate Fellow, David is recognized for his significant contributions to research on transportation energy and related issues. The award will be presented to David at TRB's annual meeting in January.
- Congratulations to PEEPSRC's John M. Miller, Lixin Tang, Curt Ayers, and Tim Burress for their contributions to a 3rd quarter review of a new motor technology being developed under ARPA-E Rare Earth Alternatives in Critical Technologies program with project lead QM Power Inc. The review's success has secured project funding through 2014.
- ORNL was well represented at the recent DOE Vehicle Technologies Directions in Engine-Efficiency and Emissions Research conference, with 7 podium presentations and 14 poster presentations–more than any other national laboratory. Special thanks to all who participated or provided support!
- Phil Maziasz of ORNL's Materials Science & Technology Division was awarded the 2012 William Hunt Eisenman Award of ASM International at the annual ASM Awards Dinner on Oct. 9 in Pittsburgh. The Eisenman recognizes "unusual achievements in industry in the practical application of materials science and engineering through production or engineering use." Phil was cited for "outstanding success in the development of new heat-resistant stainless steel and alloys with significant commercial impact in advanced transportation, coal-fired generation, and nuclear power generation." Phil's R&D efforts at ORNL span more than 37 years.
- On November 16, UT-Battelle, LLC will present its annual Awards Night honors for outstanding employees. In the category of Science Communicator, FEERC's Brian West will be honored for his sustained commitment to sharing research expertise and for his passion for educating the general and non-automotive technical communities on the details of transportation energy use, especially with respect to the potential impact of biofuels.

## Visits & Events

ORNL is hosting the DOE Vehicle Technologies Program FY13 Kickoff Meeting for Advanced Power Electronics and Electric Motors R&D, November 13-15, at the ORNL Conference Center. Approximately 100 representatives from universities, industry, and national laboratories performing R&D for the program are expected to attend the invitation-only meeting.

As America seeks to revitalize its manufacturing sector, lightweighting vehicles with low-cost carbon fiber represents a tremendous market opportunity. In early October, ORNL hosted the third meeting of the Oak Ridge Carbon Fiber Consortium, which now counts 44 member companies. The Carbon Fiber Technology Facility impressed them, new collaborations are in the works, and working groups are gaining traction.


In late September, CTA and the Sustainable Transportation Program hosted DOT visitors including Venkat Pindiprolu, Federal Transit Administration, and Peter Chipman, Research and Innovative Technology Administration. Tours were provided to the Fuels, Engines and Emissions Research Center; the Power Electronics and Electrical Machinery Research Center; the Battery Manufacturing Facility; the Vehicle Systems Integration laboratory; and the Manufacturing Demonstration Facility. Presentations on the Intelligent Transportation System deployment tracking tool, the medium and heavy truck and bus duty cycle data collection and analysis program, and the Climate Change Science Institute were provided in the Transportation Analysis and Visualization Laboratory. While at ORNL, Pindiprolu and Chipman also participated in a CTA Project Meeting on "Greenhouse Gas Emissions Calculator Incorporating Electric Vehicle Options" that is being sponsored by the Federal Transit Administration.

ORNL will host a unique workshop, November 15–16, at the ORNL Conference Center followed by tours of the National Transportation Research Center campus. The workshop is designed to gauge the state-of-the-art capabilities and opportunities in wide band gap research and development as applied to automotive traction drive applications. Organizers are expecting around 40 representatives from the wide band gap industry, universities, and national laboratories.

## Looking Ahead

ORNL is co-organizing a SAE symposium on the potential benefits of higher octane gasolines in the marketplace and the potential synergies posed by RFS biofuel requirements and CAFE regulations. The symposium will explore the gasoline regulatory environment and the opportunities for higher octane fuels to promote engine efficiency as well as challenges and opportunities in achieving higher octane ratings in the marketplace. The symposium will be held January 28 and 29 at the Washington, DC Convention Center.

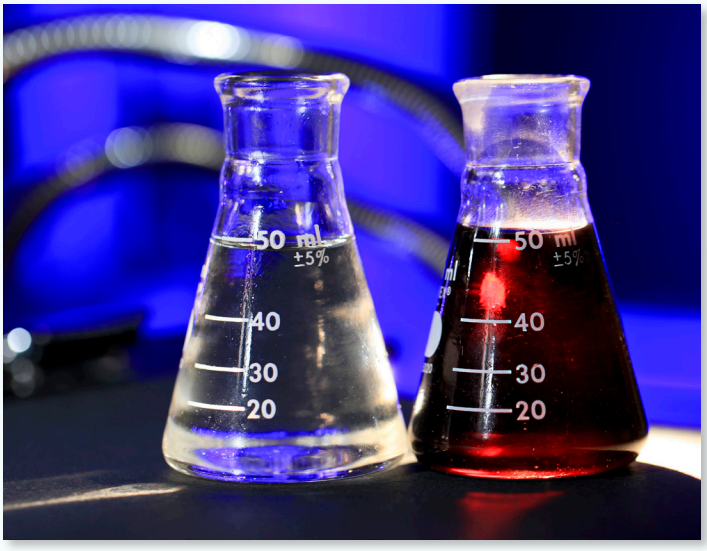
ORNL is co-organizing a SAE symposium on the opportunities of natural gas in the transportation sector. This meeting will include perspectives from the U.S. government, automobile and engine manufacturers, fleet operators, as well as energy and infrastructure providers. The meeting will be held March 12–13, at the Clemson University International Center for Automotive Research (ICAR).

## New industry collaborations

- "Conductive Polymeric Additives for Improved Lithium-Ion Battery Capacity at High Discharge Rates" is a new ORNL project getting under way with industry partner Plextronics inside the Battery Manufacturing Facility. Researchers will be exploring the Plextronics-developed material Plexcore as an additive and/or replacement for the binder found in lithium-ion cells. Project scope includes supporting preparation of electrode dispersion, electrode coating and drying, coin and pouch cell assembly, and evaluation of cell performance. Total budget is $275K over 15 months.

- DOE recently announced that a collaboration between Robert Bosch LLC, Clemson University's Center for Automotive Research, and ORNL will receive $2.7M in funding to develop an oxygen-sensor-based technique for measuring exhaust gas recirculation (EGR) levels to a level of accuracy not currently possible. EGR is a critical technology for emissions control in compression-ignition engines and is a near-term technology for improving fuel efficiency in spark-ignited engines. The award was a result of collaboration among the three entities in response to a competitive DOE FOA. FEERC researchers will lead ORNL efforts, providing experimental support to the partnership to validate modeling results and investigate sensor performance.

- ORNL hosted a kickoff meeting in August to launch a cooperative research and development agreement (CRADA) between UT-Battelle, LLC, and Shell Global Solutions (US) to develop and demonstrate oil-soluble ionic liquids as engine oil additives to improve the mechanical efficiency of internal combustion engines. The CRADA is in support of a Broad Agency Announcement award through the Vehicle Technologies Program's fuels and lubricants research area. In addition to signing the CRADA, Shell officials received overviews and tours of facilities at the National Transportation Research Center and the main campus.




*Synthetic polyalphaolefin base oil (left) and 0W10 racing lubricant containing 3% ionic liquid.*

Do you have news or information you would like to share?

Please submit to Kathy Graham,
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